Structure and Peculiarities of Fluctuations in Deeply Supercooled Water

T.V. Lokotosh and N.P. Malomuzh
Dept. of Theoretical Physics
Odessa State University
2 Dvorjanskaya str.
Odessa, 65026, Ukraine

A satisfactory description of the temperature anomalies of thermodynamic properties and kinetic coefficients of water is possible only by adequate accounting of the water structure. With suitable accuracy this can be accomplished with the help of the H-bond density n_H per molecule and the tetrahedricity parameter χ, which, in general, is a tensor of the second rank. In equilibrium, n_H and χ are functions of temperature T and pressure P. However, for weakly nonequilibrium states, $n'_H = n_H - n_H(P,T)$ and $\chi' = \chi - \chi(P,T)$ are independent and form an additional set of hydrodynamic variables. The respective system of hydrodynamic equations is proposed.

The character of equilibrium and nonequilibrium fluctuations of the main hydrodynamic variables in normal and supercoooled states is investigated. The microinhomogeneous (cluster) structure of water is taken into account. The possible types of phase diagrams of water near its spinodal are considered. It is shown that the fluctuations remain on their usual level almost up to the nearest vicinity of spinodal. Due to this, in X-ray and molecular light scattering experiments the singularities were not observed.

Modifications of the water phase diagram for the cases of finite cooling rates are studied. The possibility for the appearance of high-density and low-density water is considered. The quasithermodynamic properties of water in these states are discussed.